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AN ALGORITHM FOR COMPUTING THE STATIONARY DISTRIBUTION OF A DISCRETE-TIME BIRTH-AND-DEATH PROCESS WITH BANDED INFINITESIMAL GENERATOR

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An Algorithm for Computing the Stationary Distribution of a Discrete Birth-and-Death Process with Banded Infinitesimal Generator

TECHNICAL REPORT: NPS-MA-95-003

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Abstract

We develop an algorithm for computing approximations to the stationary distribution of a discrete birth-and-death process provided that the infinitesimal generator is a banded matrix. We begin by computing stationary distributions for processes whose infinitesimal generators are Hessenberg. Our derivation in this special case is different than the classical one but leads to the same result. We then show how to extend these ideas to get approximations when the infinitesimal generator is banded (or half-banded).

1 Introduction

A birth and death process is characterized by a population of individuals whose number changes according to the outcome of two other stochastic processes consisting of births which increase the population and deaths which decrease the population. The transition probabilities for these two processes can, in general, depend on both time and population size. The model for this stochastic dynamical system is usually described by a master equation for the transition probability for population size at a given time.

Let $N(t)$ denote the population size at time t and define the transition probability for $N(t)$ as $P(n,t) = \Pr\{N(t) = n | N(t') = n'\}$. The transition probabilities for births and deaths are usually modeled as Markovian processes by assuming that

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$$
\begin{aligned}
r(n,t) &= \Pr\{N(t+dt) = k+1 | N(t) = k\} \\
l(n,t) &= \Pr\{N(t+dt) = k-1 | N(t) = k\}
\end{aligned}
$$

where dt represents the fundamental time unit. Time can be treated as either a discrete or continuous variable. In many situations it is reasonable and convenient to model these transition probabilities as being time independent and to assume that the probability that more than a single birth or death occurs in the fundamental time unit is zero. With these assumptions the master equation for $P(n,t)$ can be written

$$
\begin{aligned}
P(n,t+dt) &= r(n-1)P(n-1,t) + l(n+1)P(n+1,t) + \\
&+ \left[1 - (r(n) + l(n))\right] P(n,t)
\end{aligned} \tag{1}
$$

The first approach to investigating 1 is to assume that

$$\lim_{t \to \infty} P(n,t+dt) - P(n,t) = 0$$

and write the equation for the stationary transition probabilities, $p(n)$, the probability that the population will eventually stabilize at n individuals, as

$$0 = -(r(n) + l(n))p(n) + r(n-1)p(n-1) + l(n+1)p(n+1) \tag{2}$$

This *stochastic balance equation* leads to the *infinitesimal generator* for the discrete time Markov process which has the following stationary distribution

$$p(n) = p(0) \prod_{j=1}^{n} \frac{r(j-1)}{l(j)} \tag{3}$$

In this paper we develop an algorithm for computing the solution to this problem and show how it can be generalized to compute approximate solutions for birth-and-death processes where both multiple births and multiple deaths can occur in the fundamental time unit. These methods are developed by converting stochastic balance equations like 2 to matrix form and applying techniques from linear algebra.

The virtue of the linear algebra approach is twofold. First, the use of finite precision calculations in linear algebra is well understood and many algorithms have been developed that can control the ill effects of round-off and other errors. Second, generalizations of the simple birth and death model give rise to generalizations of the master equations 1 and 2 for which solutions are not known. In this case, the methods we develop are still applicable. To motivate what follows, we now show how 3 results from solving an appropriate linear system.

2 A Matrix Formulation

We are interested in finding the stationary distribution $p(n)$ which satisfies equation 2. We begin by converting 2 to matrix form. In what follows vectors will be denoted by lower-case bold Roman letters and will be assumed to be column vectors. We shall denote by $\mathbf{0}$ the vector of all zeros, by $\mathbf{e}$ the vector of all ones, and by $\mathbf{e}_i$ the i'th axis vector, a vector whose i'th element is one and all others are zero. The sizes of these vectors, when they appear, shall be taken from context.

To proceed, we represent the stationary distribution $p(n)$ as an infinite column vector $\mathbf{p}$ whose i'th element $p_i = p(i-1)$ where $i = 1, 2, ..., \infty$. Note that if there were a maximum population size N then $\mathbf{p}$ would be an element of $\Re^{N+1}$. In general, however, this is not the case.

The infinitesimal generator matrix Q^T is an infinite tridiagonal matrix with entries

$$Q^T_{i,j} = \begin{cases} -(r(i-1) + l(i-1)) & \text{if } i = j \\ r(j-1) & \text{if } i - 1 = j \\ l(j-1) & \text{if } i + 1 = j \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

With these definitions, equation 2 becomes

$$Q^T \mathbf{p} = \mathbf{0} \tag{5}$$

And we see that Q^T must be rank-deficient and $\mathbf{p}$ in its null-space (or equivalently, $\mathbf{p}$ is an eigenvector of Q^T associated with the eigenvalue $\lambda = 0$). Equation 5 implies that any element of the null-space of Q^T solves the equation. To get the stationary distribution we normalize using the law of total probability, so that $\mathbf{e}^T \mathbf{p} = 1$.

3 Truncated Solutions

It is not generally possible to solve infinite systems of equations, or find eigenvectors of infinite matrices, so we consider truncating the infinite system of equations. Graphically, we truncate the infinite system by by partitioning it in the following way

$$\left[\begin{array}{cccc|ccc} \times & \times & 0 & & & & \\ \times & \ddots & \ddots & \ddots & & & \\ 0 & \ddots & & \times & & & \\ & \ddots & \times & \times & \times & & \\ \hline & & & \times & \times & \times & \\ & & & & \times & \ddots & \ddots \\ & & & & & \ddots & \\ & & & & & & \end{array}\right] \left[\begin{array}{c} p(0)\\ p(1)\\ \vdots \\ p(n-1) \\ \hline p(n) \\ \vdots \end{array}\right] = \mathbf{0}$$

and then dropping all but the first n equations.

Letting Q_n^T be the first principal $n \times n$ sub-matrix of Q^T, and $\mathbf{p}_n$ be the first principal n vector of $\mathbf{p}$, we get

$$Q_n^T \mathbf{p}_n = -l(n)p(n)\mathbf{e}_n$$

In effect, this is a matrix representation of the first n equations from 5. Letting $\mathbf{p}_n = l(n)p(n)\mathbf{f}_n$ and rearranging yields

$$Q_n^T \mathbf{f}_n = -\mathbf{e}_n \tag{6}$$

So, provided that Q_n^T is non-singular and that $l(n)p(n) \neq 0$, we can solve directly for a scalar multiple of the truncated stationary distribution $\mathbf{p}_n$.

In particular, the truncated infinitesimal generator matrix is

$$Q_n^T = \begin{bmatrix} -r(0) & l(1) & & & \\ r(0) & -r(1)-l(1) & l(2) & & \\ & r(1) & & \ddots & \\ & & \ddots & & l(n-1) \\ & & & r(n-2) & -r(n-1)-l(n-1) \end{bmatrix}$$

and has the following explicit LU factorization

$$L = \begin{bmatrix} -1 & & & \\ 1 & \ddots & & \\ & \ddots & -1 & \\ & & 1 & -1 \end{bmatrix} \qquad U = \begin{bmatrix} r(0) & -l(1) & & \\ & r(1) & \ddots & \\ & & \ddots & -l(n-1) \\ & & & r(n-1) \end{bmatrix}$$

To find the stationary distribution we solve, in succession, the triangular systems

$$\begin{aligned} L\mathbf{z}_n &= -\mathbf{e}_n \\ U\mathbf{f}_n &= \mathbf{z}_n \end{aligned}$$

Since L is unit lower triangular we see that $\mathbf{z}_n = \mathbf{e}_n$ (indeed, in general one need only know U) and $\mathbf{f}_n$ is just the solution of

$$U\mathbf{f}_n = \mathbf{e}_n$$

Backward substitution yields

$$\mathbf{f}_n = \left[\frac{l(1)l(2)...l(n)}{r(0)r(1)...r(n)}, \quad \frac{l(2)l(3)...l(n)}{r(1)r(2)...r(n)}, \quad ..., \quad \frac{l(n)}{r(n-1)r(n)}, \quad \frac{1}{r(n)}\right]^T$$

This implies that

$$p(k) = p(n+1) \prod_{j=k+1}^{n+1} \frac{l(j)}{r(j-1)} \tag{7}$$

Setting $k = 0$ and rearranging yields

$$p(n+1) = p(0) \prod_{j=1}^{n+1} \frac{r(j-1)}{l(j)}.$$

which is a well-known formula for the stationary distribution.

Note that this formula does not give the values of the stationary distribution since it involves the unknown scaling factor $p(0)$. However, it does allow us to determine, exactly, the shape of the stationary distribution. We can make a common approximation to the stationary distribution in the following way. Assume that S is the probability that the population size is less than n. Then $\mathbf{e}^T\mathbf{p}_n = S$ and hence

$$\mathbf{p}_n = \frac{S}{\mathbf{e}^T\mathbf{f}_n}\mathbf{f}_n$$

In practice, one takes n to be large so that S is close to 1. Then

$$\mathbf{p}_n \approx \frac{1}{\mathbf{e}^T\mathbf{f}_n}\mathbf{f}_n$$

4 Populations with Multiple Births

Now consider populations in which multiple births can occur. Although one approach to problems of this type is to re-scale the birth rate, $r(n)$, in some appropriate way and solve the single step problem, it is not difficult to derive the solution using traditional methods. We show that, as before, the matrix approach gives the formal solution when solved analytically.

Let $r(n,k)$ be the rate at which births of k individuals occur given that the population size is n. Equation 2 becomes

$$0 = -\left(\sum_{k=1}^{\infty} r(n,k) + l(n)\right)p(n) + \sum_{k=1}^{n} r(n-k,k)p(n-k) + l(n+1)p(n+1) \quad (8)$$

The infinitesimal generator is an infinite lower Hessenberg matrix whose elements are given by

$$Q^T_{i,j} = \begin{cases} -(\sum_{k=1}^{\infty} r(i,k) + l(i)) & \text{if } i = j \\ r(j, i-j) & \text{if } i > j \\ l(j) & \text{if } i+1 = j \\ 0 & \text{otherwise} \end{cases} \quad (9)$$

The truncated system has the same form as before except that Q^T is now lower Hessenberg instead of tridiagonal. In particular, letting $\mathbf{p}_n = l(n)p(n)\mathbf{f}_n$ we have

$$Q_n^T\mathbf{f}_n = -\mathbf{e}_n \quad (10)$$

As before, we only need to know U from the LU factorization of Q^T to find $\mathbf{f}_n$. In block form, the factorization of the truncated infinitesimal generator matrix, an $n \times n$ lower Hessenberg matrix, looks like

$$\begin{bmatrix} 1 & \mathbf{0}^T \\ \frac{1}{\alpha}\mathbf{r} & \hat{L} \end{bmatrix} \begin{bmatrix} \alpha & \beta\mathbf{e}_1^T \\ \mathbf{0} & \hat{U} \end{bmatrix} = \begin{bmatrix} \alpha & \beta\mathbf{e}_1^T \\ \mathbf{r} & \hat{Q^T} \end{bmatrix}$$

Where $\hat{L}\hat{U}$ is the LU factorization of the Schur complement which is an $n-1 \times n-1$ lower Hessenberg matrix. In particular

$$\hat{L}\hat{U} = \hat{Q^T} - \frac{\beta}{\alpha}\mathbf{r}\mathbf{e}_1^T$$

Note that U is an upper bidiagonal matrix whose first super-diagonal has elements $U_{i,i+1} = l(i)$. Let $\sigma_i = U_{i,i}$ be the diagonal elements, these can be found sequentially in the following way.

$$\begin{aligned} \sigma_1 &= \sum_{k=1}^{n} r(0,k) \\ \rho_{1,k} &= \frac{r(0,k)l(1)}{\sigma_1} \qquad k = 1,2,...,K \end{aligned}$$

And

$$\begin{aligned} \sigma_{i+1} &= \sum_{k=1}^{n} r(i,k) + l(i) - \rho_{i,1} \\ \rho_{i+1,k} &= \frac{r(i,k) - \rho i - 1, k+1}{\sigma_{i+1}} l(i) \qquad k = 1,2,...,n-1 \\ \rho_{i+1,n} &= \frac{r(i,n)}{\sigma_{i+1}} l(i) \end{aligned}$$

The final form of U is

$$U = \begin{bmatrix} \sigma_1 & -l(1) & & \\ & \sigma_2 & \ddots & \\ & & \ddots & -l(n-1) \\ & & & \sigma_n \end{bmatrix}$$

Solving by backward substitution yields

$$p(k) = p(n+1) \prod_{j=k+1}^{n+1} \frac{l(j)}{\sigma_j}$$

And setting $k = 0$ and rearranging yields

$$p(n+1) = p(0) \prod_{j=1}^{n+1} \frac{\sigma_j}{l(j)}$$

5 Processes with Multiple Births and Multiple Deaths

In the cases considered so far, the infinitesimal generator matrix is lower Hessenberg and the solution algorithms are equivalent with the classical *solution by recursion* algorithm for finding truncated solutions. The derivations we have shown are different than the classical approach but are useful because they will allow us to look at more general birth and death models in a natural way. We now consider a process in which both multiple births and multiple deaths are allowed. We will assume that jumps as large as $\pm K$ occur in both directions (it is straightforward to extend what follows to processes where the maximum possible number of births is not the same as the maximum possible number of deaths). The stochastic balance equation is

$$0 = \sum_{k=1}^{K} \{-(r(n,k) + l(n,k))p(n) + r(n-k,k)p(n-k) + l(n+k,k)p(n+k)\} \tag{11}$$

The infinitesimal generator matrix is banded, with half-bandwidth K, and of the form

$$Q^T_{i,j} = \begin{cases} -\sum_{k=1}^{K}(r(i,k) + l(i,k)) & \text{if } i = j \\ r(j, i-j) & \text{if } i > j \\ l(j, j-i) & \text{if } i < j \\ 0 & \text{otherwise} \end{cases} \tag{12}$$

The truncated system can be written

$$Q^T_n \mathbf{p}_n + S^{(n)} \mathbf{p}^{(n)} = \mathbf{0}$$

where $\mathbf{p}^{(n)} = \begin{bmatrix} p(n) & p(n+1) & \dots & p(n+K-1) \end{bmatrix}^T$ and $S^{(n)} \in \Re^{n \times K}$ has elements

$$S_{i,j}^{(n)} = \begin{cases} l(j, j+n-i) & \text{if } i \geq n-K+j-1 \\ 0 & \text{otherwise} \end{cases}$$

We shall call $S^{(n)}$ the *homogeneous complement* of Q_n^T in Q^T.

Rearranging the truncated system yields

$$Q_n^T \mathbf{p}_n = -S^{(n)} \mathbf{p}^{(n)}$$

Now, let F be the solution to

$$Q_n^T F = -S^{(n)}$$

Then $\mathbf{p}_n = F\mathbf{p}^{(n)}$ and we see that $\mathbf{p}_n$ is in the range of F. If F is rank one then we can get bp_n up to an unknown scaling. This is the essence of solution by recursion since in those cases F surely has rank one.

Based on the preceding analysis, we propose the following algorithm to find $p(0), p(1), ...p(N_0)$ for a birth and death process that can have from 1 to K deaths in each time step. We assume that $N_0 > K$.

1. Let $n = N_0$.
2. Using the truncated infinitesimal generator Q_n^T and its homogeneous complement $S^{(n)}$ solve $Q_n^T F_n = -S^{(n)}$.
3. Compute the singular value decomposition of F_n, that is $U \Sigma V^T = F_n$
4. Construct the approximation $\mathbf{p}_n \approx \alpha \mathbf{u}_1$ where α is some unknown constant and $\mathbf{u}_1$ is the first column of U.
5. If $\sigma_1^{(n)}$, the largest singular value of F_n is sufficiently greater than $\sigma_2^{(n)}$ then stop and accept the approximation. Otherwise set $n := n+1$ and return to step 2.

It is possible to update F_n and it's singular value decomposition quickly.

6 A More General Formulation

The method that has been developed above can be put into a much more general framework. We begin by noting that any Markov process whose infinitesimal generator is banded is a Quasi-Birth-Death (QBD) process. Provided we choose the block size correctly (it must be no less than the bandwidth) the infinitesimal generator can be written as a block tridiagonal matrix

$$Q^T = \begin{bmatrix} D_0 & A_1 & & & \\ B_1 & D_1 & A_2 & & \\ & \ddots & \ddots & \ddots & \end{bmatrix}$$

If we partition $\mathbf{p} = \begin{bmatrix} \pi_0 & \pi_1 & \dots \end{bmatrix}^T$ so that it is compatible for block multiplication, then the stochastic balance equations can be written in the following form

$$D_0\pi_0 + A_1\pi_1 = \mathbf{0}$$

and

$$B_i\pi_{i-1} + D_i\pi_i + A_{i+1}\pi_{i+1} = \mathbf{0}$$

for $i = 1, 2, \dots$

There are two common approaches to problems of this type. First, if the Markov process represented by this matrix is *nearly completely decomposable* (NCD), that is, if the off-diagonal blocks are sufficiently small in some sense, one can disregard them and assume the Markov chain is completely decomposable (some justification for this can be found in [3]). Then π_i are solutions to $D_i\pi_i = \mathbf{0}$ and can be solved for individually. This yields approximations to the segments of $\mathbf{p}$ which must then be carefully assembled to get the stationary distribution (see [4] for a beautiful treatment of these methods). The problem with this approach is that it is hard to tell how good the approximations to the π_i are since it is not clear what effect disregarding the A_i and B_i will have on the solution.

A second approach is stochastic complementation ([2]). This method also computes the segments π_i but does so exactly using block Gaussian elimination. This method does not throw anything away so it is exact (at least on paper). Unfortunately, the method is quite costly.

Our method can be extended quite naturally to this more general framework. In particular, given the block tridiagonal Q^T shown above, we define the homogeneous complement of D_i in Q^T to be $S_i = \begin{bmatrix} \hat{B}_{i-1} & \hat{A}_i \end{bmatrix}$, where $\hat{A}_i$ is a matrix composed of only the non-zero columns of A_i, $\hat{B}_i$ is defined similarly, and B_0 is taken to be a zero matrix. We then solve

$$D_i F_i = -S_i$$

and approximate π_i with the left singular vector associated with the largest singular value of F_i. This is a simple process and allows us to estimate of the quality of our approximations by examining the ratios of the largest and second largest singular values of each F_i. This method is embarassingly parallel.

We can use this method to generate a starting guess for those algorithms known generally as *Iterative Aggregation/Disaggregation* (IAD). These are efficient multi-grid like methods and include the well-known KMS [1] and Takahashi [5] algorithms. We can also develop an adaptive variation by using the algorithm of section 5 to solve for π_0 first. We then apply this same algorithm to solve for each succesive segment using the more general definition of the homogeneous complement. This allows us to vary the block sizes adaptively so that each estimate of a segment will be a good one. This approach lacks parallelism but would give both an initial guess and a partitioning for IAD algorithms.

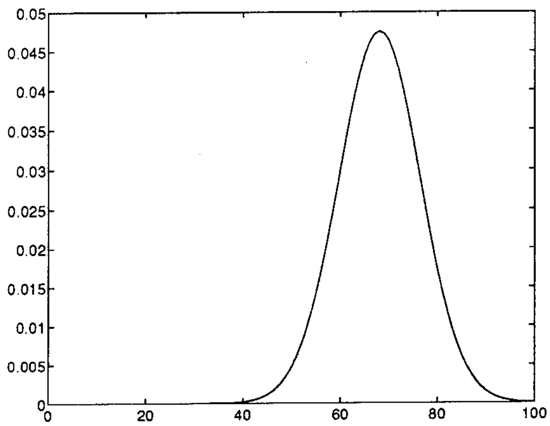
7 An Example

As an example we look at a simple birth-and-death process in which as many as two births or deaths can occur in the fundamental time unit. The specific model we will look at is characterized by the following transition rates

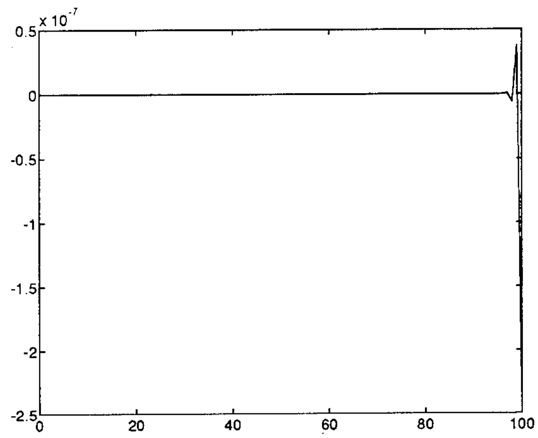
$$\begin{aligned} r(n,1) &= 0.237(n+1)e^{-0.0165n} \\ r(n,2) &= 0.105(n+1)e^{-0.0231n} \\ l(n,1) &= 0.088n \\ l(n,2) &= 0.018n \end{aligned}$$

Notice that there is a positive birth rate even when the population size is zero. This migration term is necessary so that 0 is not an absorbing state which would preclude the existence of a stationary probability vector.

Analytically, we need to find the null-vector of the full infinitesimal generator Q, an infinite matrix. In practice it is sufficient to find the eigenvector associated with the smallest magnitude eigenvalue of Q_n. As n gets large, this eigenvector should converge to the stationary distribution, after appropriate normalization. For this example, when $n = 200$ the smallest eigenvalue has magnitude roughly 10^{-13} and we see good convergence of the eigenvector. Of course, we had to solve a large eigenvalue problem to get this approximation. Below is a plot of the first 100 elements of the eigenvector (past 100 the distribution dies out)

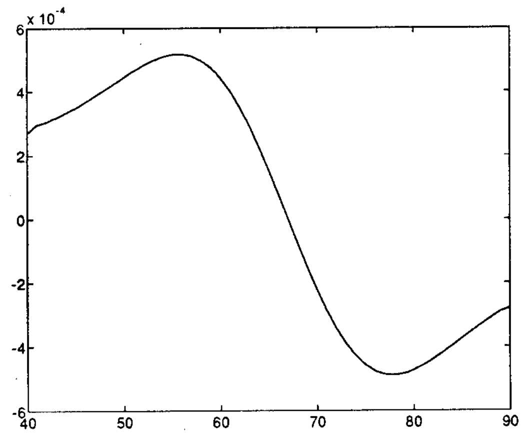


We now explore the application of the methods described in this paper to this example. First of all, working with the matrix truncated to the first 100 equations we take the homogeneous complement, solve and return the left singular vector associated with the largest magnitude singular value. The ratio of the largest to the second largest singular value is roughly 3×10^5. The approximation is almost identical to that found by solving a full 200×200 eigenproblem. Below is a plot of the difference between the approximations after appropriate normalization.

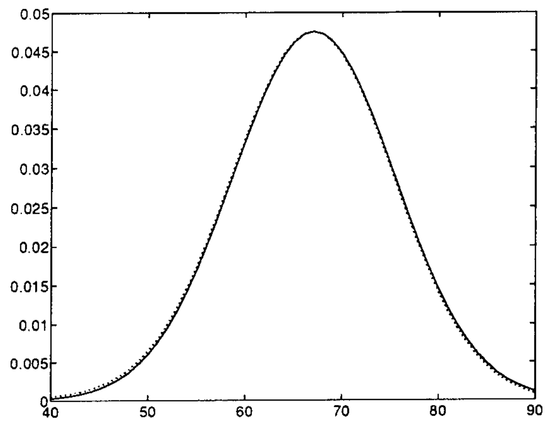


Notice that the difference never exceeds 2.5×10^{-7} in magnitude. Moreover, the relative error in the approximation for all n such that $p(n) > .005$ never exceeds 3×10^{-12}. Note also that we did not have to solve a 200×200 eigenproblem to get this solution. We only had to solve a single linear system, with a 100×100 matrix and a 100×2 right hand side, and compute the singular value decomposition of a 100×2 matrix.

If we truncate the infinitesimal generator so that it covers population sizes ranging from 40 to 90 only we find that the ratio of the two largest singular values of F is roughly 36.4. After appropriate normalization, the difference between this segment and the full solution is always less than 6×10^{-4}, we see this plotted below.



And finally we show a plot of the computed segment (dotted line) with the segment from the full solution.



We see that the method works quite well in this case and is much less costly since the SVD computation involves a very small matrix.

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